Dimethyl decanedioate

	,					
106-79	9-6	DT.	XSI	010	267	40

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.08

Global applicability domain: Inside

Local applicability domain index: 5.31e-01

Confidence level: 5.82e-01

Nearest Neighbors from the Training Set

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2,2-Dimethylpropane-1,3-diyl bis(2-methylprop-2-enoate)

Measured: 2.79 **Predicted:** 2.66

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2-Pyrrolidinone, 1-hexyl-

Measured: 2.60 Predicted: 2.28

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Geranyl acetate Measured: 4.04 Predicted: 4.14

Image not found

cis-3,7-Dimethyl-2,6-octadien-1-

yl acetate

Measured: 4.04 Predicted: 4.20

Image not found

Heptyl acetate
Measured: 3.46
Predicted: 3.40